CONFIGURATION SPACE THREE-BODY SCATTERING THEORY*

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ARPA Contract DA-31-124-ARO-D-440 and NASA Grant NGR-39-011-035

THESIS

Abstract. Results are quoted for the "physical" three-body transition operator yielding the volume-independent three-body reaction coefficient, in terms of which one computes the three-body elastic scattering rate when three initially free independently moving particles collide under the influence of short range forces.

Consider the scattering of three particles $\alpha = 1, 2, 3$ which for the purposes of this work may be considered elementary, spinless and distinguishable. A major objective of the theory is to determine the physical three-body reaction coefficient

$$\bar{w}(i\to f) \equiv \bar{w}(\vec{k}_i\to\vec{k}_f) \equiv \bar{w}(\vec{k}_{1i},\vec{k}_{2i},\vec{k}_{3i} \to \vec{k}_{1f},\vec{k}_{2f},\vec{k}_{3f})$$

expressing the probability of three-body elastic scattering in the laboratory system, from initial momenta $\hbar\vec{k}_{\alpha i} = m_\alpha \vec{v}_{\alpha i}$ to final momenta $\hbar\vec{k}_{\alpha f}$. The reaction coefficient $\bar{w}$ is related to observation by

$$\hat{w}(\vec{k}_i\to\vec{k}_f) = N_1 N_2 N_3 \tau \bar{w}(\vec{k}_i\to\vec{k}_f)$$

where $\hat{w}d\vec{k}_{1f}d\vec{k}_{2f}d\vec{k}_{3f}$ is the observed number of scatterings per unit time into wave number ranges $d\vec{k}_{1f}, d\vec{k}_{2f}, d\vec{k}_{3f}$ in a (large) volume τ containing N_α particles α per unit volume moving with the precise velocities $\vec{v}_\alpha$. Presumably $\hat{w}/\tau$ should be independent of τ, i.e., presumably in a correctly formulated theory the computed reaction coefficient $\bar{w}$ will be independent of τ.

If only by analogy with known results[1,2] for collisions between two incident bodies, one expects that

$$\bar{w}(\vec{k}_i \to \vec{k}_f) = \hbar^{-1}(2\pi)^{-5} \mid \bar{T}^t(\vec{k}_i \to \vec{k}_f)\mid^2 \delta(E_f - E_i)\delta(\vec{K}_f - \vec{K}_i)d\vec{k}_{1f}d\vec{k}_{2f}d\vec{k}_{3f} \qquad (1)$$

where E and $\hbar\vec{K}$ are respectively the total energy and momentum in the laboratory system, and where

$$\bar{T}^t(\vec{k}_i \to \vec{k}_f) \equiv \langle f|\bar{T}^t|i\rangle = \bar{\psi}_f^* \, \bar{T}^t \, \bar{\psi}_i$$

is the center-of-mass system matrix element of the "physical" three-particle transition operator $\bar{T}^t$ between initial and final plane wave states $\bar{\psi}$. A determinative definition of[3] T^t is not immediately apparent. What is apparent is that [granting the validity of Eq. (1)] the physical transition operator T^t must differ from the customarily employed "total" transition operator

$$T(E) = V - V[G^{(+)}(E)]V$$

where V is the total interaction and $G^{(+)}$ is the outgoing total Green's function. The center-of-mass system matrix elements

$$\langle f|\bar{T}|i\rangle = \bar{\psi}_f^* \cdot \bar{T} \, \bar{\psi}_i \qquad (2)$$

contain δ-functions[4,5] [in addition to those already appearing in Eq. (1)] which -- when directly inserted into (1) -- make the right side of (1) proportional to the squares of δ-functions, i.e., make (1) mathematically meaningless. Reinterpretation of the squared δ-functions along lines[2] which yield sensible results for reaction coefficients in two-body collisions, e.g.,

$$[\delta(\vec{K}_f-\vec{K}_i)]^2 = (2\pi)^{-3}\delta(\vec{K}_f-\vec{K}_i)\int d\vec{R}\,\exp[\,i(\vec{K}_i-\vec{K}_f)\cdot\vec{R}]$$
$$= (2\pi)^{-3}\delta(\vec{K}_f-\vec{K}_i)\int d\vec{R} \cong (2\pi)^{-3}\tau\,\delta(\vec{K}_f-\vec{K}_i) \quad (3)$$

would lead to a three-body $\bar{w}$ depending on the volume τ, i.e., to an inconsistency with the presumption that the number of three-body scattering events in τ should be strictly proportional to τ in the limit $\tau\to\infty$. Thus the center-of-mass matrix elements $\langle f|\bar{T}^t|i\rangle$ must not contain the δ-functions present in (2).

The foregoing assertions have motivated me to seek a configuration space derivation of Eq. (1) and of a closed form expression for T^t. Some of the results[6] of this quest are quoted below, without proof.[7] A configuration space approach has been adopted because: (i) derivations of Eq. (1) in the literature[8] do not distinguish between T and T^t, and customarily are couched essentially ab initio in the momentum representation (which also happens to be the most natural representation for utilization of diagrammatic methods); (ii) previous investigations[2] have shown that formulating scattering theory in configuration space can be both useful and instructive. In their totality the configuration space results obtained do furnish a welcome confirmation of the general correctness of the customary momentum space procedures, which usually attain their goals [e.g., a derivation of Eq. (1)] much more rapidly than do configuration space procedures. Of course, this confirmation would be gratuitous were it not for the facts that the configuration space and momentum space formulations each involve some questionable mathematical manipulations, after starting from equally questionable by no means obviously identical physical assumptions. In essence, the work on three-three elastic scattering reported here can be considered to be a first step in the direction of deducing correct formal expressions for three-three reactions between composite systems; in the field of chemistry such reactions are important and often measurable.

Let

$$\Psi_i^{(+)}(E) = \psi_i(E) + \phi_i^{(+)}(E) \tag{4}$$

be the properly and uniquely specified [e.g., via the Faddeev equations[9]] solution to Schrödinger's equation describing the collision between particles 1,2,3 in the initial plane wave state

$$\psi_i(E) = \exp\left[i(\vec{k}_{1i}\cdot\vec{r}_1 + \vec{k}_{2i}\cdot\vec{r}_2 + \vec{k}_{3i}\cdot\vec{r}_3)\right] \equiv \exp\left[i\ \vec{k}_i\cdot\vec{r}\ \right]$$

where, for simplicity, it is supposed that all forces are short range. Define $\bar{\Phi}_i^{t(+)}(\vec{r};\bar{E})$ to be that part of $\bar{\Phi}_i^{(+)}(\vec{r};\bar{E})$ which behaves asymptotically like the center-of-mass system free space Green's function

$$\bar{G}_F^{(+)}(\vec{r}_1,\vec{r}_2,\vec{r}_3\ ;\vec{r}_1{}',\vec{r}_2{}',\vec{r}_3{}'\ ;\bar{E}) \equiv \bar{G}_F^{(+)}(\vec{r};\vec{r}\,';\bar{E})$$

when $\vec{r}_1,\vec{r}_2,\vec{r}_3$ each approach infinity in such a fashion that no $\vec{r}_{\alpha\beta} = \vec{r}_\alpha - \vec{r}_\beta$ remains finite. Then I assume that the physical three-body elastic scattering is described by $\bar{\Phi}_i^{t(+)}(\bar{E})$. Now, computing the contribution made by $\bar{\Phi}_i^{t(+)}$ to the center-of-mass system outgoing probability current [which determines the reaction coefficient in the time-independent configuration space formulation of scattering theory] one finds Eq. (3) holds, with $\bar{T}^t(\vec{k}_i\to\vec{k}_f)$ given by

$$\lim_{r\to\infty||\vec{\nu}_f} \bar{\Phi}_i^{t(+)}(\vec{r};\bar{E}) = -\,C_2(\bar{E})\,\frac{e^{i\bar{\rho}\sqrt{\bar{E}}}}{\bar{\rho}^{5/2}}\,\bar{T}^t(\vec{k}_i\to\vec{k}_f)\quad . \tag{5}$$

In (5), $\vec{\nu}_f$ denotes a direction -- in the nine-dimensional configuration space subtended by $\vec{r}_1,\vec{r}_2,\vec{r}_3$ -- along which no $\vec{r}_{\alpha\beta}$ remains finite as every $\vec{r}_\alpha = r_\alpha\vec{n}_{\alpha f}$ approaches infinity, where $\vec{n}_{\alpha f}$ is the direction of $\vec{r}_\alpha$ in physical space; $\vec{\nu}_f$ is specified by $\vec{n}_{\alpha f}$ and the limiting ratios r_α/r_β. The final momenta $\hbar\vec{k}_{\alpha f}$ are in turn specified by $\vec{\nu}_f$, lie along $\vec{n}_{\alpha f}$, and have their expected magnitudes for scattering into directions $\vec{n}_{\alpha f}$. Furthermore,

$C_2(\bar{E})$ is a known constant, depending on $\bar{E}$ and the particle masses m_α, while

$$(m_1+m_2+m_3)\bar{\rho}^2 = 2\hbar^{-2}(m_1 m_2 r_{12}^2 + m_2 m_3 r_{23}^2 + m_3 m_1 r_{31}^2) \quad .$$

The scattered wave $\Phi_i^{(+)}$ in (4) can be written in the form

$$\Phi_i^{(+)} = \Phi_{12}^{(+)} + \Phi_{23}^{(+)} + \Phi_{31}^{(+)} + \Phi_{23}^{s(+)} + \Phi_{31}^{s(+)} + \Phi_{12}^{s(+)} + \Phi_i^{d(+)} \tag{6}$$

where

$$\Phi_{12}^{(+)} = -(H_{12}-E-i\varepsilon)^{-1} V_{12}\psi_i(E) \quad , \text{ etc.}$$

$$\Phi_{23}^{s(+)} \equiv \Phi_{2331}^{(+)} + \Phi_{2312}^{(+)} = -(H_{23}-E-i\varepsilon)^{-1} V_{23} [\Phi_{31}^{(+)} + \Phi_{12}^{(+)}] \text{ , etc.} \tag{7}$$

The quantity $\Phi_{12}^{(+)}$ is the laboratory system scattered wave when particles 1,2,3 collide in the absence of interactions other than $V_{12}(\vec{r}_{12})$; in other words, $\Phi_{12}^{(+)}$ is that part of $\Phi_i^{(+)}$ which is associated with the bubble diagram of Fig. 1a. The corresponding center-of-mass system $\bar{\Phi}_{12}^{(+)}(\vec{r})$ has a plane wave factor in configuration space, denoting the fact that during the collision represented by Fig. 1a particle 3 moves with constant velocity relative to the center of mass of the entire 1,2,3 system. Therefore no parts of $\bar{\Phi}_{\alpha\beta}^{(+)}$ behave asymptotically like the everywhere outgoing $\bar{G}_F^{(+)}(\vec{r};\vec{r}';\bar{E})$ as $\vec{r} \to \infty \,||\, \vec{v}_f$, i.e., no parts of $\bar{\Phi}_{\alpha\beta}^{(+)}$ should be included in $\bar{\Phi}_i^{t(+)}$.

The quantities $\Phi_{\alpha\beta}^{s(+)}$ in (6) are the parts of $\Phi_i^{(+)}$ associated with double-scattering bubble diagrams; for example, the $\Phi_{2312}^{(+)}$ term in (7) is associated with the diagram of Fig. 1b. It can be shown that the corresponding $\bar{\Phi}_{2312}^{(+)}(\vec{r})$ contains contributions behaving like $\bar{\rho}^{-2}$ as $\vec{r} \to \infty \,||\, \vec{v}_f$; therefore $\bar{\Phi}_i^{t(+)}$ cannot include all parts of $\bar{\Phi}_{\alpha\beta}^{s(+)}$, because $\bar{G}_F^{(+)}(\vec{r};\vec{r}') \sim \bar{\rho}^{-5/2}$ as $\vec{r} \to \infty \,||\, \vec{v}_f$. On the other hand, $\bar{\Phi}_{2312}^{(+)}(\vec{r})$ also contains contributions behaving like $\bar{\rho}^{-5/2}$ as $\vec{r} \to \infty \,||\, \vec{v}_f$, and these should be included in $\bar{\Phi}_i^{t(+)}$. The remaining $\Phi_i^{d(+)}$ contribution to $\Phi_i^{(+)}$ is associated with the set of all triple (e.g., Fig. 1c) and higher order bubble diagrams. It can be seen that $\bar{\Phi}_i^{d(+)}(\vec{r})$ behaves asymptotically like $\bar{G}_F^{(+)}(\vec{r};\vec{r}\,')$ as $\vec{r} \to \infty \,||\vec{v}_f$, except along an inconsequential subset $\vec{v}_f^{\,\prime}$ of lower dimensionality (than the 5-dimensional manifold spanned by $\vec{v}_f$).

It now can be concluded that the physical transition amplitude $\bar{T}^t(\vec{k}_i \to \vec{k}_f)$ includes all matrix elements corresponding to triple and higher order bubble diagrams. In addition, $\bar{T}^t(\vec{k}_i \to \vec{k}_f)$ includes the matrix elements corresponding to the double-scattering bubble diagrams of type Fig. 1b, if and only if each two-particle scattering fails to conserve energy, i.e., if and only if the intermediate state (located in Fig. 1b at the dashed line) lies off the energy shell. In other words, the parts of $\bar{\Phi}_{2312}^{(+)}(\vec{r})$ behaving like $\bar{\rho}^{-2}$ as $\vec{r} \to \infty \,||\vec{v}_f$ are associated with those bubble diagrams Fig. 1b for which the intermediate state lies on the energy shell, i.e., for which the individual bubbles in Fig. 1b represent actual (because they are energy-conserving) two-particle scatterings; of course, momentum always is conserved in each bubble (two-particle scattering) in Fig. 1b. The matrix elements corresponding to the various diagrams in Fig. 1 are computed in accordance with the usual rules.[4,5] In particular, the contribution of Fig. 1b to $\bar{T}^t(\vec{k}_i \to \vec{k}_f)$ is

$$\ddot{T}^t_{2312}(\vec{k}_i \to \vec{k}_f) = -\frac{2\mu_{12}}{\hbar^2}\,\frac{\langle\vec{k}_{23f}|t_{23f}|\vec{B}\rangle\langle\vec{A}|t_{12i}|\vec{k}_{12i}\rangle}{A^2 - k_{12i}^2} \tag{8}$$

where μ_{12} is the reduced mass of 1, 2; t_{12i} is the purely two-body transition operator for scattering of particles 1,2 evaluated at energy $E_{12i} = \hbar^2 k_{12i}^2/2\mu_{12}$, and similarly for t_{23f}; $\mu_{12}(\vec{v}_1 - \vec{v}_2) = \hbar\,\vec{k}_{12}$, etc.; and $\vec{A}$, $\vec{B}$, which denote momentum vectors in the intermediate state, are completely specified by the given initial and final momenta $\vec{k}_i, \vec{k}_f$. At $A^2 = k_{12i}^2$, the intermediate state in Fig. 1b lies on the energy shell, and the right side of (8) is replaced by zero.

If order of integration and $\lim \vec{r} \to \infty \,||\, \vec{v}_f$ could be interchanged in $(H_{23}-E-i\varepsilon)^{-1} V_{23} \Phi_{12}^{(+)}$, the scattered wave contribution $\bar{\Phi}_{2312}^{(+)}(\vec{r})$ would behave like $\bar{G}_F^{(+)}(\vec{r};\vec{r}')$ as $\vec{r} \to \infty \,||\, \vec{v}_f$, because in this limit $\bar{G}_{23}^{(+)}(\vec{r};\vec{r}') \equiv (\bar{H}_{23}-\bar{E}-i\varepsilon)^{-1}$ behaves asymptotically like $\bar{G}_F^{(+)}(\vec{r};\vec{r}')$. Obviously this interchange must be unjustified, since we already know $\bar{\Phi}_{2312}^{(+)}(\vec{r})$ does not behave asymptotically like $\bar{G}_F^{(+)}(\vec{r};\vec{r}')$. If the interchange is performed nevertheless, one obtains the obvious analogue of (5), which analogue defines the contribution $\bar{T}_{2312}(\vec{k}_i \to \vec{k}_f)$ made to $\bar{T}(\vec{k}_i \to \vec{k}_f)$ by the $\bar{\Phi}_{2312}^{(+)}$ part of $\bar{\Phi}_i^{(+)}$. One finds $\bar{T}_{2312}(\vec{k}_i \to \vec{k}_f)$ is precisely the usual matrix element associated with the diagram Fig. 1b; when written in configuration space this matrix element is seen to contain a contribution proportional to $\delta(k_{12i}^2 - A^2)$. The same δ-function contribution is obtained if one returns to the original momentum representation formula (8) for this matrix element — wherein $A^2 - k_{12i}^2 - i\varepsilon$ replaces $A^2 - k_{12i}^2$ in the denominator — and makes the conventional reinterpretation[10] of $\lim (A^2 - k_{12i}^2 - i\varepsilon)^{-1}$ as $\varepsilon \to 0$ when $A^2 = k_{12i}^2$. This one-dimensional δ-function contribution to $\bar{T}(\vec{k}_i \to \vec{k}_f)$, if inserted into (1) and reinterpreted along the lines (3), would yield a contribution to $\hat{w}$ proportional to $\tau^{4/3}$; a simple geometrical argument shows this is precisely the τ-dependence one expects to observe if the experimentalist measuring the three-body scattering rate does not so arrange his apparatus that actual double scattering events are excluded. In other words, in the configuration space approach an unwanted $\delta(k_{12i}^2 - A^2)$ contribution to $\bar{T}^t(\vec{k}_i \to \vec{k}_f)$ is obtained only because a mathematically unjustified manipulation has been performed; however, the result of this unjustified manipulation turns out to have a physically sensible interpretation. The same remarks can be made concerning other divergent expressions which arise in the configuration space formulation of scattering theory; in general these divergences arise because of invalid mathematical operations, but lead to physically interpretable results nevertheless.

Finally I note that the Faddeev reformulation of the Lippmann-Schwinger equation in no way mitigates the reaction rate prediction complications associated with the double-scattering diagrams Fig. 1b. In fact, if the Faddeev equations[9] are written in the form [using Faddeev's notation in essence]

$$\phi^{(1)} = -G_{23}V_{23}\psi_i - G_F T_{23}[\phi^{(2)} + \phi^{(3)}] , \quad \text{etc.}$$

then it can be seen that

$$-G_F\{T_{23}[\phi^{(2)} + \phi^{(3)}] + T_{31}[\phi^{(3)} + \phi^{(1)}] + T_{12}[\phi^{(1)} + \phi^{(2)}]\} = \phi_{23}^{s(+)} + \phi_{31}^{s(+)} + \phi_{12}^{s(+)} + \phi_i^{d(+)} .$$

FOOTNOTES

*Supported by the Advanced Research Projects Agency under Contract No. DA-31-124-ARO-D-440 and by the National Aeronautics and Space Administration Grant No. NGR-30-011-035; the research was completed during the author's tenure as a Visiting Fellow at the Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado.

1. A. Messiah, Quantum Mechanics (Wiley, 1962), Vol. II, p. 806.
2. E. Gerjuoy, Ann. Phys. **5**, 58 (1958).
3. Barred and unbarred symbols regularly will denote corresponding quantities in the center-of-mass and laboratory systems respectively.
4. Cf., e.g., S. Weinberg, Phys. Rev. **135**, B232 (1964).
5. K. M. Watson and J. Nuttall, Topics in Several Particle Dynamics (Holden-Day, San Francisco, 1967), Chap. 4.

6. Early results have been reported in the Proceedings of the International Conference on Three-Body Collisions, Birmingham, England, July 8-10, 1969.

7. The detailed analysis leading to these results is much too long to be reproduced here, and will have to be published elsewhere.

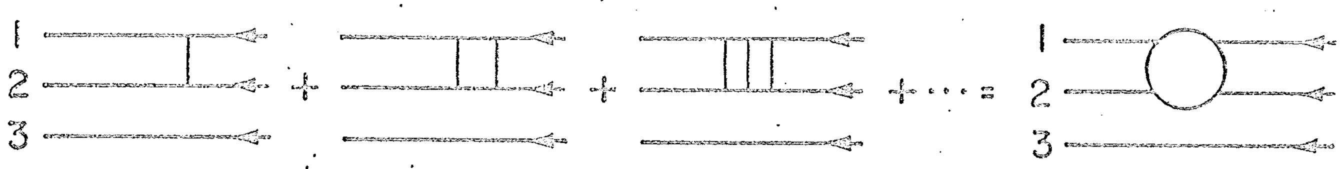
8. B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950); M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953); W. Brenig and R. Haag, "General Quantum Theory of Collision Processes," in Quantum Scattering Theory edited by Marc Ross (Indiana University Press, Bloomington, Indiana, 1963), p. 13.

9. L. D. Faddeev, Soviet Phys. JETP **12**, 1014 (1961).

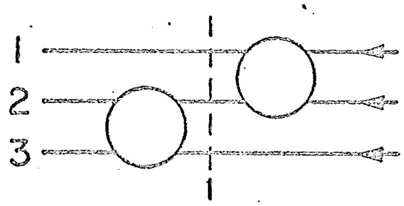
10. W. Brenig and R. Haag, ibid., pp. 106-108.

FIGURE CAPTION

Fig. 1. Scattering diagrams: (a) two-particle scattering between 1, 2 wherein 3 is present but non-interacting; (b) double scattering, first between 1, 2 and then between 2, 3; (c) a typical triple scattering diagram.



(a)



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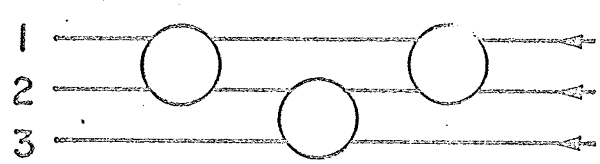

(c)